Method for innovative synthesis-design of chemical process flowsheets

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Abstract

Chemical process synthesis-design involve the identification of the processing route to reach a desired product from a specified set of raw materials, design of the operations involved in the processing route, the calculations of utility requirements, the calculations of waste and emission to the surrounding and many more. Different methods (knowledge-based [1], mathematical programming [2], hybrid, etc.) have been proposed and are also currently employed to solve these synthesis-design problems. D' Anterroches [3] proposed a group contribution based approach to solve the synthesis-design problem of chemical processes, where, chemical process flowsheets could be synthesized in the same way as atoms or groups of atoms are synthesized to form molecules in computer aided molecular design (CAMD) techniques [4]. That, from a library of building blocks (functional process-groups) and a set of rules to join them, chemical process flowsheets are generated and evaluated for properties like energy consumption, atom efficiency, environmental impact, etc., using functional process-group based property models. In this way, a list of feasible chemical process flowsheets are quickly generated, screened and selected for further analysis. In the next stage, the design parameters for the operations of the flowsheet are established through reverse engineering approaches based on driving forces available for each operation. In the final stage, when all the necessary information for a rigorous process simulation is available, rigorous simulation is performed to validate the synthesis-design. Note that since the flowsheet is synthesized and the operations in the flowsheet designed to match a set of design targets, there are no iterations involved as the final flowsheet is among the best, if not the best.

In this paper, the implementation of the computer-aided process-group based flowsheet synthesis-design framework is presented together with an extended library of flowsheet property models to predict the environmental impact, safety factors, product recovery and purity, which are employed to screen the generated alternatives. Also, new process groups are added to represent unit operations for applications in bio-processes. The implemented framework in the form of a new computer-aided tool in ICAS (Integrated Computer Aided System) will be highlighted through two case studies, one involving the synthesis of a chemical process flowsheet (the well-known Hydrodealkylation of toluene process) and another for a biochemical process flowsheet (production of ethanol from lignocellulose). In both cases, not only the reported designs are found and matched, but also new innovative designs are found, which is possible because of the predictive nature of the models used and the synthesis of flowsheets through the group contribution approach.

These case studies and others developed to test the method, the framework and the ICAS-tool help to confirm their applicability, scope and significance, since it is possible to find new and better alternatives not reported earlier. The application-examples also focus on the use of SFILES notation system, developed specially for the process-group based synthesis-design method, to store and/or visualize the structural information of any process flowsheet represented by process-groups. As an extension, the SFILES notation is extended to store the process information through which representation of flowsheet alternatives for rigorous process simulation (for example, with an external process simulator) would be possible.

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